HARTREE-FOCK EXCHANGE WITH LOCALIZED ORBITALS FOR FAST AND EFFICIENT CALCULATIONS WITH QUANTUM ESPRESSO CODE

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A new method is proposed and validated for the calculation of the Hartree-Fock exchange with plane waves. The method, based on the recently proposed Adaptively Compressed Exchange approach, exploits the orbital localization for reducing the computational burden of the exchange calculations.
Such a method has been tested on different systems and a significant speed up in the calculations with respect to preexisting approaches has been found. On the other side, the accuracy of the electronic structure and molecular properties remains relatively high.
In this talk the theoretical framework of the method will be presented, with a particular focus on the implementation in Quantum ESPRESSO, computational performances and accuracy of the chemico-physical properties.